

4π models of CMEs and ICMEs

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Abstract Coronal mass ejections (CMEs), which dynamically connect the solar surface to the far reaches of interplanetary space, represent a major manifestation of solar activity. They are not only of principal interest but also play a pivotal role in the context of space weather predictions. The steady improvement of both numerical methods and computational resources during recent years has allowed for the creation of increasingly realistic models of interplanetary CMEs (ICMEs), which can now be compared to high-quality observational data from various space-bound missions. This review discusses existing models of CMEs, characterizing them by scientific aim and scope, CME initiation method, and physical effects included, thereby stressing the importance of fully 3-D (4π) spatial coverage.

Keywords: Coronal mass ejections: initiation and propagation, Coronal heating theory, Magnetohydrodynamics, Solar Wind: disturbances.

1. Introduction

Coronal mass ejections (CMEs) are one of the most spectacular manifestations of solar activity. Their mass and energy output, insignificant as they may seem when compared to the Sun as a whole, are still able to severely distort planetary magnetospheres even after they have been diluted considerably during an expansion phase covering a distance of one AU or more, thus bringing the solar influence to the outermost reaches of interplanetary space.

CMEs also relate to many other fields of solar and stellar physics. They are intimately linked to flares (*e.g.* Shanmugaraju, Moon, and Vršnak, 2011, and references therein), and often give rise to strong shock fronts, which act as efficient accelerator engines for solar energetic particles (*e.g.* Reames, 1999). It has also been recognized that CMEs play an important role for the restructuring of the Sun's global magnetic field over the course of the solar cycle (Schwadron, Owens, and Crooker, 2008).

Apart from these motivations to understand the CME phenomenon from a purely scientific perspective, it has also become apparent in recent years that the increasing complexity of modern technology, in particular communication

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infrastructure, has also led to an increased vulnerability of this technology to the adverse effects of *space weather*. The resulting commercially-driven demand for high-precision forecasting tools has given a continuing boost to research efforts in the field (Baker, 2002; Pulkkinen, 2007, and references therein). Besides the ensuing increased public interest in the subject, timely advances in computing hardware and numerical algorithms have allowed for the development of sophisticated large-scale models of CME dynamics, which are the subject of this review. The paper is structured as follows. After this introduction, Section 2 will discuss ways in which the vast spectrum of existing CME models can be categorized, with special focus on their specific strengths and possible weaknesses. Section 3 describes how different types of models can be validated against observations, and Section 4 presents a concluding summary and a modest suggestion for further action to improve on the comparability of results from different models.

1.1. What makes CME modeling a demanding task?

To realistically model the evolution of a CME is a very demanding task for several reasons:

1. The CME phenomenon spans vast temporal and spatial scales. Even disregarding the microphysics involved in, *e.g.*, flare reconnection (some 10^{-8} s, several meters) best described with kinetic approaches, a CME's life cycle from pre-eruption (when it extends over a small fraction of a solar radius R_{\odot}) to interplanetary expansion and finally merging with features like global interaction regions at the far reaches of the heliosphere extends over some six orders of magnitude in space and time, see Forbes *et al.* (2006) and in particular Figure 1 therein. For this reason, existing fluid-based models usually specialize on either initiation/eruption, interplanetary expansion, or interaction with corotating interaction regions, planetary magnetospheres, or other CMEs.
2. Even single CMEs show great variety in their morphology. Although during solar minimum, many of them originate from streamer blowouts and often exhibit the famous three-part "light bulb" structure consisting of a bright, semi-spherical front enclosing a dark cavity and a bright core (Illing and Hundhausen, 1986), the situation changes towards solar maximum; CME events then usually originate from active regions and tend to exhibit a much more irregular structure, which can differ markedly from the three-part textbook configuration. Even for prominence-related CMEs, the appearance of the three-part structure depends on the prominence location (Cremades and Bothmer, 2004). The fraction of CMEs that cannot be classified into the subgroup of 'magnetic clouds' (Burlaga *et al.*, 1981) was estimated to be near 2/3 by Gosling (1990), albeit with a marked variation throughout the solar cycle from almost none during some years of minimum up to $\sim 60\%$ at maximum (Li *et al.*, 2011). See Kilpua *et al.* (2011) for a recent review on magnetic cloud models and related multipoint observations. In their sample of almost 1,000 CMEs, Howard *et al.* (1985) were able to identify as many as ten morphological classes, and even this list is probably still far from exhaustive. On top of this, the large angular width of CMEs ($\approx 50^\circ$ on average, see St. Cyr *et al.*

- (2000)), combined with their high rate of occurrence especially during solar maximum, makes interaction among them likely, thus giving rise to an even wider spectrum of possible morphologies.
3. Attempts to reproduce observed events tend to be severely under-determined from observational side. To fully constrain a well-posed magnetohydrodynamic (MHD) model, initial and boundary conditions for density, pressure, and the velocity and magnetic field vectors must be specified; yet the initial (pre-eruptive) conditions are poorly known and usually rely on surface magnetograms and coronagraph images to constrain the magnetic field structure, possibly complemented by *in situ* observations at individual locations.
 4. CME propagation is an inherently three-dimensional (3-D) process. Even if the CME initially exhibits some form of spatial symmetry, its ensuing expansion in a complex magnetic environment will in any case break that symmetry, rendering modeling approaches with implied spatial symmetries problematic (see Section 2.2.3).

2. Model classifications

Both the complexity and the enormous range of scales covered by the CME phenomenon make it necessary to devise separate models to address the different stages of CME evolution, most notably the onset and eruption, the ensuing phase of propagation and expansion, and a possibly following interaction with other structures (planetary magnetospheres, other CMEs).

2.1. Modeling CME onset...

Since the kinetic energy of a CME is in most cases greater than what the photosphere can provide during the timespan of the eruption, all current models for the initiation phase assume a slow accumulation of energy, followed by its rapid release due to loss of equilibrium. Existing analytical models for this early phase are few in number and have to rely on simplifying assumptions to keep the calculations manageable.

In the 2-D ideal MHD model of Forbes and Isenberg (1991), the magnetic energy of an initially stable filament is slowly increased by converging advection of additional flux until a current sheet forms. Reconnection below the filament can then lead to a 'catastrophe', *i.e.*, a sudden loss of mechanical equilibrium which causes the filament to erupt. Lin *et al.* (1998) extended this model and considered a finite curvature along the invariant direction (thereby transforming the infinitely long cylindrical filament into a force-free toroidal flux rope around the Sun). While both models predict eruption as soon as the stored magnetic energy exceeds a certain threshold, the now finite curvature force was shown to yield a qualitatively different behavior, which now favors eruption for large flux ropes.

Early numerical approaches to the simulation of solar eruptions relied on relatively simple 2-D arcade geometries, in which a forced shearing motion of the structure footpoints was employed to generate slow CMEs by driving the system

past a critical point in its parameter space (*e.g.* Mikic, Barnes, and Schnack, 1988; Steinolfson, 1991).

The currently considered scenarios for CME outbreak largely fall into the following groups:

1. The *mass loading* model relies on the notion that within a prominence, the equilibrium between magnetic tension and the gravity force of the mass above the structure allows for the slow accumulation of more mass, which merely causes the prominence to bend downwards under the increased weight of its load (Fong, Low, and Fan, 2002; Zhang and Low, 2004). Eruption can occur when some restructuring of the magnetic field causes part of the material to suddenly drain away, causing a loss of equilibrium. These authors distinguish 'normal' and 'inverse' prominences based on their orientation with respect to the background field, and find that the normal variant is more likely to erupt. This finding has been confirmed numerically by Chané *et al.* (2006), see Section 3.1.
2. *Flux cancellation* models (also known as 'catastrophe models') start with a (usually twisted) arch-shaped flux rope which undergoes reconnective flux cancellation (Martin, Livi, and Wang, 1985) at its neutral line. This increases both the tube twist and its magnetic pressure at the expense of the overlying field, thus moving the equilibrium position to greater heights until eruption occurs because no further neighboring equilibrium exists. Notable numerical investigations of this process were carried out, in increasing order of complexity, by, *e.g.*, Amari *et al.* (2000), Linker *et al.* (2003), and Roussev *et al.* (2004).
3. *Tether cutting* (Moore *et al.*, 2001) is very similar to flux cancellation, except maybe more impulsive and at slightly larger photospheric heights, cf. Chen (2011). It starts with a single closed bipole (essentially a magnetic arcade) consisting of a twisted sigmoidal core and an 'envelope' of less twisted field lines. If the core axis is suitably aligned with respect to the neutral line, reconnection below the axis will weaken the tension of the envelope. This causes the core part to move upwards, thereby stretching the envelope field and leading to even more reconnection in the current sheet thus formed below until confinement becomes too weak to prevent the core from erupting. The model agrees well with x-ray images from the *Soft X-ray Telescope* (SXT) on board *Yohkoh*, but is deemed implausible on the basis of energy considerations (Antiochos, DeVore, and Klimchuk, 1999).
4. The *breakout model* (Antiochos, DeVore, and Klimchuk, 1999) starts with a quadrupolar arcade featuring an external X-type null point. The arcade is sheared and/or twisted by footpoint motions until the null is deformed into a current sheet at which reconnection sets in. This removes some of the overlying flux, which widens the current sheet further, thus leading to a runaway process which eventually causes the arcade to erupt. This model's crucial feature is that the ejected plasmoid is topologically detached from the arcade right from the beginning, which is a favorable condition to avoid the Aly-Sturrock constraint (Aly, 1984; Sturrock, 1991), see below. Corresponding MHD simulations have been carried out by MacNeice *et al.* (2004) and Lynch *et al.* (2004).

5. Finally, two different variants of the *MHD kink instability* have been proposed as possible initiation mechanisms. Using the analytic field by Titov and Démoulin (1999) as initial configuration, Török and Kliem (2005) showed that if this flux rope is twisted beyond a critical value, the twist is partially transformed into writhe, and a helical MHD kink instability sets in, as was already hinted at by an earlier stability analysis (Hood and Priest, 1981). This may or may not lead to an eruption, depending on the strength of the overlying field (*e.g.* Fan, 2005; Rachmeler, DeForest, and Kankelborg, 2009). The kink instability thus not only addresses and explains the sudden release, but also the previous storage of magnetic energy, and can furthermore explain some related observations such as soft x-ray sigmoids (Török, Kliem, and Titov, 2004). Second, Kliem and Török (2006) analyzed the stability of a torus-shaped current loop against radial perturbations and the possibly ensuing torus instability, which they described as "a lateral kink instability distributed uniformly over the ring." They found that this instability may trigger the onset of a self-accelerating expansion along the major radius that can explain both the eruption of a flux rope (when treated as the upper half of a torus whose lower half is submerged below the photosphere) and the ensuing acceleration behavior of different types of CMEs, notably slow and fast ones.

Common features of the last four models are the formation of a twisted flux rope and the generation of a current sheet below the flux rope. What sets the first and last model apart from the others is that they rely on purely ideal MHD effects, and do not involve any reconnection (at least not as a trigger element). Reconnection has been viewed as a convenient means to circumvent the Aly-Sturrock constraint according to which any process which entirely opens a force-free field to infinity would in fact increase the overall magnetic energy and therefore could not drive an eruption. However, Forbes *et al.* (2006) enumerate several other avenues to avoid the constraint (such as fields being non-force-free, not simply connected, or containing field lines disconnected from the Sun). Additionally, Rachmeler, DeForest, and Kankelborg (2009) used a Lagrangian simulation scheme with no (numerical or physical) resistivity whatsoever to demonstrate that reconnection is not necessary to drive fast CME eruptions. This theoretical finding is corroborated by the small but non-zero number of observed fast CMEs showing no sign of flare association (Marqué, Posner, and Klein, 2006). More details about the initiation and early propagation phase of CMEs, especially of those originating from helmet streamers and prominences, can be found in the reviews by Low (1996), Forbes (2000), and Vršnak (2008), as well as in Chapter 8 of Howard (2011).

Recently, Lin, Gallagher, and Raftery (2010) analyzed the relevance of some of the above-mentioned mechanisms for the kinematic evolution of two CME events and found the breakout and catastrophe models to yield the best agreement with their derived time profiles of height, velocity, and acceleration. This is reminiscent to speculations by Howard (2011) suggesting that "...it is likely that different types of CMEs are best described by different models. Indeed, it is possible that most, if not all of the models [...] may be appropriate to describe some CMEs under certain conditions."

2.2. ...and propagation

2.2.1. Trajectory mapping

For the purpose of space weather forecasts, the three most crucial quantities to be delivered by a model are the CME's trajectory, travel time, and geo-effectiveness. To a first approximation, expansion is radial, implying that only halo CMEs are likely to hit Earth. Schwenn *et al.* (2005) found the respective rates of false and missing alarms for this correlation to be 15 and 20 percent, which underlines the need for more sophisticated approaches. A first correction is the tendency of the Parker spiral magnetic field to cause a slight westward deflection for fast CMEs, and a stronger eastward deflection for the slower ones (Wang *et al.*, 2004). From a sample of 841 CME observations using the *Large Angle and Spectrometric Coronagraph* (LASCO) on board the *Solar and Heliospheric Observatory* (SOHO) mission, St. Cyr *et al.* (2000) found 14% of them to exhibit clear indication of non-radial motion.

Observationally derived trajectories are often ambiguous because coronagraph images suffer from projection effects, and the frequencies of the type II radio bursts associated with an eruption only provide the source heliocentric distance (which furthermore depends on the assumed electron density profile). Coronagraph data from the *Solar Terrestrial Relations Observatory* (STEREO) mission (Kaiser, 2005) can be used for stereoscopic reconstruction from image pairs (Howard and Tappin, 2008). This, however, is a well-defined problem only for curve-like objects (Inhester, 2006), while for extended, diffuse objects like CMEs, some ambiguity remains. This is usually resolved by manual identification of those points in image pairs which are assumed to belong to the same point-like feature in physical space; since this procedure uses two 2-D points to determine a single 3-D point, it is in fact an *over-defined* problem. For the small sample investigated by Maloney, Gallagher, and McAteer (2009), these authors found their derived trajectories to be consistent with quasi-radial expansion.

2.2.2. Simple kinematic models

Several authors have tried to deduce a CME's travel time T in which it covers a distance $R_{s/c}$ as a function of its initial velocity v_0 by fitting formulas like

$$v_0 T + a T^2 / 2 = R_{s/c} \quad (1)$$

to (v_0, T) data pairs from actual events, thus using the required acceleration a (due to thermal pressure, magnetic forces, gravity, momentum conservation ("snow plough effect", Tappin, 2006), and aerodynamic drag) as a free parameter. Gopalswamy *et al.* (2001) found a minimum variation of $\Delta T \approx 10$ h for their sample if $a = 0$ beyond 0.75 AU. The tentative inclusion of a drag term $a(v) \propto (v - v_{sw})^2$ (Cargill, 2004) was shown to have little influence on the method performance, though it is indeed observed that for large distances, the CME speed will approach the speed v_{sw} of the ambient medium (Lindsay *et al.*, 1999; Maloney, Gallagher, and McAteer, 2009). Relating these empirical $T =$

$T(v_0)$ formulas to observed events yields large discrepancies, which can be attributed to the inherent oversimplification of this method. Therefore, it has to be concluded that both the CMEs themselves and the interplanetary medium which they encounter are much too variable and structured for simple fitting laws of this kind to yield more than rough estimates.

As an intermediate step between one-parameter fitting and fully self-consistent MHD simulations, spatially resolved kinematic models such as the HAF model (Hakamada and Akasofu, 1982; Fry, 1985) have been used to predict the arrival times of shocks and the spatial structure of the inner heliosphere as it is modulated by corotating interaction regions. This model projects a (possibly time-dependent) boundary condition at $2.5R_{\odot}$ outwards along stream lines, and has been calibrated using direct (albeit only 1-D) MHD simulations (Sun *et al.*, 1985).

2.2.3. Numerical MHD propagation models

The numerical study of propagating CMEs is a challenging task mainly because the need to track structures with details smaller than a solar radius across at least 1 AU requires very high spatial resolution. On top of that, the configuration has no apparent symmetry properties that could be exploited to reduce computational expenses. During solar maximum, the Sun's global magnetic field is inherently 3-D, and even during solar minimum, CMEs are never observed to travel along the Sun's polar axis, thus breaking the rotational symmetry of the field.

In the past, two strategies have been used to deal with this difficulty. The first is to ignore the misalignment of expansion direction and magnetic symmetry axis and to assume cylindrical symmetry anyway (*e.g.* Chané *et al.*, 2006). This implies a closed, torus-shaped CME geometry which is not anchored on the Sun, a configuration that could potentially be relevant for tube-shaped magnetic clouds. In their comparison of 2-D versus 3-D models, Jacobs, van der Holst, and Poedts (2007) conclude that propagation models with cylindrical symmetry, however inadequate from a principal point of view, can still provide useful and computationally inexpensive estimates, which can then be used to set up a refined and symmetry-free follow-up simulation. The general usefulness of such approaches requires that the parameters are properly transferred between both geometries, which necessarily requires several ambiguities to be resolved.

The second avenue is to use a fully 3-D model with sufficient resolution in all three coordinate directions. The resulting vast increase in computational expense can be moderated by the use of specially tailored grids, in particular spherical grid geometries with a radial mesh spacing Δr which increases with heliocentric radius r (*e.g.* Pomoell, Vainio, and Kissmann, 2011).

For a global fluid simulation of CMEs, the numerical grid must be chosen carefully to optimize the trade-off between the advantages and shortcomings of different grid geometries. While spherical, Sun-centered grids are obviously best adapted to the Sun's shape and thus greatly simplify the specification of boundary conditions and the description of predominantly radial expansion, the large variation in cell sizes may lead to undesirably low time steps, and the

necessary inclusion of the polar axis requires a delicate treatment of coordinate singularities. The latter can be avoided by the use of so-called overset grids, such as the Cubed Sphere (Ronchi, Iacono, and Paolucci, 1996) or the Ying-Yang grid (Kageyama and Sato, 2004). These, however, require some form of interpolation scheme to establish a seamless connection between the sub-grids, which usually destroys the conservative properties of the code within the interpolation region. For applications of these grids to 3-D solar wind modeling see Feng *et al.* (2010, 2011). Cartesian coordinates, which do not present such difficulties, remain popular among CME modelers for exactly this reason, although the implementation of spherical boundaries like the photosphere then either requires some form of weighted interpolation procedure (*e.g.* Kleimann *et al.*, 2009) or a much increased spatial resolution. The latter requirement becomes much less severe by the use of adaptive mesh refinement techniques (*e.g.* BATS-R-US, de Zeeuw *et al.*, 2000). Logically rectangular grids (Calhoun, Helzel, and LeVeque, 2008), which permit the smooth inclusion of curved boundaries into an otherwise Cartesian grid geometry, harbor the potential to combine the advantages of Cartesian and spherical coordinate grids, but have until now not been used in any large-scale 3-D simulation with relevance to space physics.

Another interesting approach is the use of multi-scale models (*e.g.* Riley *et al.*, 2006), which consist of a radially nested sequence of grids, such that the outer boundary condition of a given grid is fed into the next, coarser grid as an inner boundary condition of the latter. The fact that the solar wind plasma flow becomes super-Alfvénic after only a few R_{\odot} frees these authors from the requirement to run the model simultaneously on all sub-grids. The multi-scale approach is also a key feature of the *Space Weather Modeling Framework* (SWMF, see Tóth *et al.*, 2005), which condenses a total of nine model components (for the magnetosphere, inner heliosphere, radiation belts, etc.) into a modular, versatile space physics-based simulation environment.

2.3. Classification by aim and scope

Existing models for the expansion/interaction phase of CMEs largely fall into two categories:

1. 'principal' studies, which intend to investigate the relevance of a (usually small) set of free parameters on the resulting dynamics, and
2. 'realistic' simulations, which are aimed at a usable prediction of the development of actual events, and therefore need to include as much physics and data as possible.

Consequently, these two types of models differ noticeably in the way in which they implement boundary and initial conditions. On the one hand, principal models tend to use a background solar wind which is either uniform (*e.g.* Vandas, Odstrčil, and Watari, 2002; Dalakishvili *et al.*, 2011b) or moderately structured (*e.g.* Odstrčil and Pizzo, 1999; Manchester *et al.*, 2004b), combined with a dipolar, or at most quadrupolar magnetic field, and possibly amended with a planar current sheet. Realistic global-scale models, on the other hand, routinely rely on synoptic magnetograms to specify a potential coronal magnetic field as a photospheric boundary condition, from which a reasonable initial condition can be derived (*e.g.*

Hayashi, Zhao, and Liu, 2006; Lugaz *et al.*, 2007). To fully constrain this field solution, additional assumptions about the type of \mathbf{B} field need to be made, the most popular being that the field is either potential ($\nabla \times \mathbf{B} = \mathbf{0}$), linearly force-free ($\nabla \times \mathbf{B} = \alpha \mathbf{B}$), or non-linearly force-free ($\nabla \times \mathbf{B} = \alpha(\mathbf{r}) \mathbf{B}$). For a review of strategies and algorithms to obtain force-free solutions see Metcalf *et al.* (2008); a critical assessment of their performance on actual data has been presented by De Rosa *et al.* (2009).

Alternatively, vector magnetograms have been used to calculate localized non-linear force-free fields on the scale of active regions, from which CME-like eruptions can be launched in a simulation (Kataoka *et al.*, 2009). Once the magnetic field is known, empirical formulas can be used to determine suitable initial conditions for the remaining fluid quantities density, velocity, and temperature (*e.g.* Detman *et al.*, 2006).

2.4. Method of initiation

Given that the physical process which triggers an eruption is still not conclusively settled, there is some freedom in the choice of methods to numerically start this process. Density-driven models (Groth *et al.*, 2000; Chané *et al.*, 2006; Kleimann *et al.*, 2009) increase the pressure and/or density (and occasionally also the radial momentum, thereby imposing an additional mass inflow (*e.g.* Keppens and Goedbloed, 2000)) below a closed field line configuration until the inward tension of the field can no longer confine the growing internal pressure and gives way to a violent expulsion of the accumulated plasma blob. Similarly, additional magnetic flux can be artificially pushed through the photosphere (*e.g.* Fan and Gibson, 2007; Fan, 2011). Note that this latter approach must be carefully distinguished from flux emergence models, which are used to study the physical process of buoyant flux tubes emerging from the convection zone. The initial field may be further destabilized by, *e.g.*, local magnetic reconnection (*e.g.* Forbes and Priest, 1995; Chen and Shibata, 2000), or by an initial force imbalance, *e.g.* due to buoyancy. Popular initial setups of the latter kind include the self-similar expanding flux rope by Gibson and Low (1998), which has been employed by, *e.g.*, Manchester *et al.* (2004b) to initialize simulations of CMEs, just like the famous Titov-Démoulin flux rope (Titov and Démoulin, 1999).

Finally, the required instability can also be produced by shearing the photospheric footpoints of an arcade until it becomes unstable and is forced to open up spacewards. The effect of shearing motions on solar magnetic structures has been investigated theoretically (Low, 1977), observationally (Deng *et al.*, 2001), and numerically (*e.g.* Mikic and Linker, 1994; Jacobs, Poedts, and van der Holst, 2006). ■

From these methods, the density-driven one is special in that it is not supposed to mimic a process that is actually assumed to happen on the Sun; moreover, its justification lies in the pragmatic notion that if the focus is on the propagation phase, the details of initiation are of secondary importance, thus justifying the use of a method that is easy to implement and produces a relatively realistic outcome. The same rationale was also given by Pomoell, Vainio, and Kissmann (2008), who start their Cartesian 2-D simulation using a set of line currents similar to the one employed by Chen *et al.* (2002), and then apply an artificial

volume force to the interior of the detached flux rope to pull the core region upwards (which requires the trajectory of interior fluid elements to be dynamically traced during the acceleration phase).

2.5. Treatment of the energy budget

Despite almost six decades of undiminished efforts to understand the heating of the solar corona, this vital issue is still far from being settled (Cranmer, 2002; Marsch, 2006). For practical reasons, models seeking to describe a CME's propagation in the corona and inner heliosphere have to adopt a formalism to model the distribution and release of energy, which opens up another possibility to classify them.

The simplest one would be to link the plasma pressure p and mass density ρ via an adiabatic closure relation

$$p \sim \rho^\gamma . \quad (2)$$

In this case, again the simplest (albeit also the most unrealistic) choice would be to assume an (almost) isothermal plasma by setting the adiabatic index γ to unity, or a value slightly larger than unity, such as 1.05. Using the physically appropriate value of 5/3 in conjunction with Equation (2) is usually not feasible because the effect of adiabatic cooling would quickly reduce the temperature down to unrealistically low values. This problem is sometimes mediated by using a spatially varying adiabatic exponent, either as an explicitly prescribed dependence $\gamma = \gamma(\mathbf{r})$ (*e.g.* Fahr, Bird, and Ripken, 1977; Wu *et al.*, 1999), or derived from energy considerations based on the Bernoulli equation (Cohen *et al.*, 2007) or from interpreting the low value of γ close to the Sun in terms of internal energy being stored as additional degrees of freedom in large-scale turbulence (Roussev *et al.*, 2003). The obvious downside of using unphysically low adiabatic indices is the resulting inability of the model to correctly reproduce the properties of shocks, which may or may not be acceptable in a given situation, but which must in any case be kept in mind when interpreting the results thus obtained. If $\gamma = 5/3$ holds throughout the considered volume of space, a full energy equation for the total energy density e like

$$\partial_t e + \nabla \cdot [(e + p + \|\mathbf{B}\|^2/2) \mathbf{u} - (\mathbf{u} \cdot \mathbf{B}) \mathbf{B}] = (\mathbf{g} \cdot \mathbf{u} + Q)\rho \quad (3)$$

(in which \mathbf{u} denotes the flow velocity and \mathbf{g} the acceleration due to gravity) with heating source term Q has to be used. Popular choices for Q include *ad hoc* heating functions like

$$Q(\mathbf{r}) = q(\mathbf{r}) [T_0 - T] \quad (4)$$

(Manchester *et al.*, 2004b), where T_0 is a spatially dependent "target temperature", which is fine-tuned to reproduce a realistic quiet-Sun temperature distribution. The main shortcoming of this approach is that it is obviously biased towards the target temperature, or in other words, it will systematically underestimate the temperature change which is brought about by, *e.g.*, the passage of a

CME. Another, more recent approach is that of Pomoell, Vainio, and Kissmann (2011), who employ an energy equation

$$\partial_t(p/\rho^\gamma) + \mathbf{u} \cdot \nabla (p/\rho^\gamma) = S \quad (5)$$

and first run a quiet-Sun simulation using $\gamma = 1.05$ and $S = 0$ (and no CME), followed by the 'main' run using $\gamma = 5/3$ and

$$S = \mathbf{u}_1 \cdot \nabla \left(p_1 / \rho_1^{5/3} \right) \quad (6)$$

where the subscript 1 denotes values from the $\gamma = 1.05$ run. This procedure guarantees that both runs share the same stationary (quiet-Sun) state.

2.6. Alfvénic wave heating

As an alternative to the pragmatic heating functions of Section 2.5, attempts have been made to amend the underlying solar wind model with a more physical heating process. A promising candidate for such a mechanism is heating by Alfvén waves, which are generated at photospheric levels, then travel outward along magnetic field lines while being shifted towards an upper limit frequency f_h at which they dissipate and deposit their energy as heat. In its full form, this scheme requires an entire wave power spectrum $P(f, \mathbf{r}, t)$ to be modeled for each position \mathbf{r} . A dynamic equation for the temporal change of P has to be solved for each frequency f , and the waves then couple back to the MHD system via:

1. the accelerating negative gradient of the wave pressure

$$p_w \sim \int_{f_0}^{f_h} P(f) \, df \quad (7)$$

representing the magnetic pressure of the fluctuations, and

2. a wave heating term

$$Q_w = F(f_h, \mathbf{r}) - P(f_h(\mathbf{r}), \mathbf{r}) [\mathbf{u} \pm \mathbf{v}_A] \cdot \nabla f_h(\mathbf{r}) \quad (8)$$

in which the so-called cascading function $F = F(P, f)$ governs the spectral evolution of P , and \mathbf{v}_A is the local Alfvén velocity.

More details can be found in the review by Fichtner *et al.* (2008). This formalism has been successfully applied to purely radial models of the quiet-Sun solar wind (Laitinen, Fichtner, and Vainio, 2003), and appears to be a promising alternative to the phenomenological heating functions discussed in Section 2.5, although the extension to the generally more complicated magnetic field structures encountered in symmetry-free CME simulations is clearly non-trivial. First results obtained with a wave-heated solar wind model (albeit relying on the scalar wave energy densities ε_\pm parallel (+) and anti-parallel (−) to \mathbf{B} rather than the full spectral information) have been presented by van der Holst *et al.* (2010).

3. Connecting to observations

As can be expected from their very different aims, 'principal' and 'realistic' models give qualitatively different types of results; one could also say that they provide answers to different types of questions.

3.1. Selected findings from 'principal' models

Since several analytical CME models rely on the simplifying assumption of self-similarity (Farrugia, Osherovich, and Burlaga, 1995; Gibson and Low, 1998; Nakwacki *et al.*, 2008; Wang, Zhang, and Shen, 2009), it is a vital question whether this property can be confirmed numerically. Dalakishvili *et al.* (2011a) considered an idealized model for a cylindrical magnetic cloud, and numerically confirmed that an initially self-similar configuration maintains this property at later stages. Using a slightly more realistic 3-D CME model, Kleimann *et al.* (2009) compared the derived time profiles of density and magnetic field strength at different heliospheric distances, and also found indication of self-similar evolution at least in the early phase of propagation, which in this case covered a mere $10 R_{\odot}$. This is consistent with observations which show a CME's cone angle to be approximately constant in time (Schwenn *et al.*, 2005), although other simulations have been performed in which the evolution starts to depart from self-similarity after several tens of R_{\odot} (*e.g.* Manchester *et al.*, 2004a; Chané *et al.*, 2006). As was demonstrated by Riley and Crooker (2004), these findings can be reconciled by observing that the passive advection of a structure in a spherically diverging flow causes the aspect ratio (azimuthal over radial extent) of the structure to increase linearly with radial distance. A CME of initially spherical cross-section will thus tend to be flattened into a pancake-like shell, a process counteracted only by the CME's own pressure-driven expansion and its magnetic tension force, which acts towards a reduction of field line curvature and thus tends to work against excessive flattening.

Jacobs *et al.* (2005) compared several popular CME propagation models and found the resulting dynamics to be strongly dependent on both the included physics (most notably the heating mechanism) and the background wind, among other things confirming the intuitive notion that higher speeds are found in fast, dilute winds. Chané *et al.* (2006) investigated the influence of the CME's initial polarity with respect to the background field and found that 'normal' prominences result in fast, compact, approximately circular CMEs which get deflected equatorwards, while CMEs which develop from 'inverse' prominences are slower, pancake-shaped, and tend to deflect polewards, thus confirming a previous theoretical prediction by Zhang and Low (2004).

3.2. The situation for 'realistic' models

A functional prediction tool as envisaged by the space weather forecasting community would take the observed distribution of photospheric magnetic field at the instant of CME outbreak, infer from it the global initial state for all MHD variable fields, then run a detailed CME simulation from which the expected physical conditions at a given location (typically at Earth orbit) can

be extracted. Therefore, realistic models will typically try to reproduce *in situ* observations by spacecraft such as *WIND*, *Ulysses*, or the *Advanced Composition Explorer* (ACE) (see, *e.g.*, Chané, Poedts, and van der Holst, 2008). For regions closer to the Sun, another possibility to assess the predictive capabilities of the model is the creation of artificial white-light coronagraph images, which can be contrasted with actual images of the respective event, as was done by, *e.g.*, Lugaz *et al.* (2007). A first quantitative comparison of this type was presented by Manchester *et al.* (2008), who not only compared the absolute projected brightness distribution but also the derived mass and velocity of the CME in question.

While visual inspection of these comparisons often indicates impressive agreement between simulation and observation, it must however be noted that such comparisons tend to be biased towards good agreement, since publications will typically show only a few selected results from a limited parameter range, in spite of the fact that models are quite sensitive to the chosen parameters (*e.g.* Schrijver *et al.*, 2008). (For instance, Chané, Poedts, and van der Holst (2008) perform 24 different runs but explicitly state that they only show their *best fit* to the ACE data of the target event.) This makes it difficult to assess the predictive capabilities of a given model for 'real world' forecasting applications, in which *a posteriori* selection of parameter sets is not a valid option.

4. Conclusions

CMEs represent a very diverse and important class of heliospheric transients. Besides a purely scientific desire to understand their true nature, the urgent need for accurate space weather forecasts creates a strong commercially-driven incentive to intensify the study of these phenomena.

Since purely kinematic models are inadequate to capture their highly non-linear evolution, 3-D MHD simulations are indispensable to model the different stages of a CME's life cycle, with the long-term goal of providing reliable forecasts. Associated difficulties mainly concern the need for high spatial resolution — although the ever-increasing performance of computing power has helped much to mitigate this problem —, the ambiguity induced by the need to complement observational input by reasonable assumptions about the remaining quantities not obtainable from direct observation, and the fact that to this day, no universally accepted model for the initiation phase exists.

Generally speaking, the model developing community draws huge benefits from high-quality spacecraft data to: 1. constrain the initial and boundary conditions and 2. to allow for an *a posteriori* validation of the obtained simulation results. Since these results and predictions crucially depend on both the adopted initial parameters and the physical effects included in the model, more (parameter) studies are needed to quantify their respective influences. Furthermore, an unbiased comparison between different space-weather prediction tools is currently difficult because each group of authors tends to choose a different event, relies on different input data from the event in question, and sometimes also picks different methods and criteria to validate their results. It thus seems that the

community could benefit enormously from some form of standardized space weather forecasting benchmark, in analogy to community-wide benchmark test suites known from and used for the simulation of the heliosphere (Müller *et al.*, 2008) or for convection in the Earth’s interior (King *et al.*, 2010).

Acknowledgements Financial support through Research Unit 1048 (projects FI 706/8-1 and FI 706/8-2), funded by the Deutsche Forschungsgemeinschaft (DFG), is gratefully acknowledged. This work also benefitted from the EU RNT *Solaire* (MTRN-CT-2006-035484). Furthermore, the author thanks Horst Fichtner and the anonymous referee for their constructive comments.

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